

# XYZ quantum Heisenberg models with $p$ -orbital bosons

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(Dated: April 12, 2013)

We demonstrate how the spin-1/2 XYZ quantum Heisenberg model can be realized with bosonic atoms loaded in the  $p$ -band of an optical lattice in the Mott regime. The sign and relative strength of the couplings characterizing the model are demonstrated to be experimentally tuneable. We discuss the phase diagram in the one dimensional case, and show that finite size effects relevant for trapped systems lead to devil's staircase structure. Finally, we discuss experimental issues related to preparation, manipulation and detection.

PACS numbers: 03.75.Lm, 67.85.Hj, 05.30.Rt

*Introduction.*— Powerful tools developed recently to unravel the physics of many-body quantum systems offer an exciting platform for understanding quantum magnetism. It is now possible to engineer different systems in the lab that mimic the physics of theoretically challenging spin models [1], thereby performing “quantum simulations” as suggested long ago [2]. Along these lines, systems of trapped ions are promising candidates and have already been employed to simulate both small [3] and large [4] numbers of spins. In these setups, however, sustaining control over the parameters becomes very difficult as the system size increases. Furthermore, due to confining trapping potentials, realizations are limited to chains with up to 25 spins. It is also very difficult to construct paradigmatic spin models with short range interactions using systems of trapped ions.

Such obstacles are less severe for realizations of spin models with cold atoms in optical lattices [1]. A bosonic system in a deep tilted lattice has recently been used to simulate the phase transition in the 1D Ising model [5]. Fermionic atoms were employed to study dynamical properties of quantum magnetism beyond spin-1/2 systems [6], in which case the spin degrees of freedom were encoded in the internal atomic states. This idea, first introduced in Ref. [7], has also been applied to other configurations, and simulation of different types of spin models have been proposed [8]. However, due to the character of the atomic  $s$ -wave scattering among the different Zeeman levels, such mappings usually yield effective spin models supporting continuous symmetries like the XXZ model, which is invariant under  $U(1)$  transformation. But as the main goal of a quantum simulator is to realize systems that cannot be tackled via analytical and/or numerical approaches, it is important to explore alternative scenarios that yield low symmetry spin models with anisotropic couplings and external fields.

In this paper we propose such a scenario by demonstrating that bosonic atoms in the first excited band ( $p$ -band) of a two-dimensional (2D) optical lattice can

realize the spin-1/2 XYZ quantum Heisenberg model in an external field. Systems of cold atoms in excited bands feature an additional orbital degree of freedom [9] that gives rise to novel physical properties whose theoretical [10] and experimental [11, 12] aspects have been recently investigated. Their dynamics include “orbital changing” interactions, where two atoms in one of the orbital states scatter into two atoms that occupy orbital states of a different type. This is the key mechanism leading to the anisotropy of the effective spin model: These processes reduce the continuous  $U(1)$  symmetry into a set of discrete  $Z_2$  symmetries characteristic of the XYZ model. We furthermore show how the strength and sign of the couplings can be experimentally controlled. This means that one can realize a whole class of anisotropic XYZ models with ferromagnetic and/or anti-ferromagnetic correlations.

To illustrate the rich physics which can be explored with this system and to examine finite size effects relevant for the trapped systems, we discuss the phase diagram for the 1D XYZ chain. This case exhibits ferromagnetic as well as anti-ferromagnetic phases, a magnetized field-dependent state or polarized phase, a spin-flop, and a floating phase [13]. We provide an exact diagonalization of this model for a finite system relevant for the trapped case. This reveals that finite size effects result in the appearance of a devil's staircase manifested in the form of spin density waves. Finally, we discuss how to experimentally probe and manipulate the spin degrees of freedom.

*$p$ -orbital Bose system.*— We consider bosonic atoms of mass  $m$  in an optical lattice of the form  $V(\mathbf{r}) = V_x \sin^2(k_x x) + V_y \sin^2(k_y y) + V_z \sin^2(k_z z)$  with  $V_\alpha$  and  $k_\alpha$  the amplitude and wave number in the direction  $\alpha$ . Assuming that all atoms are in the first excited  $p$  orbital,

the tight-binding Hamiltonian is

$$\hat{H} = - \sum_{ij,\alpha} t_{ij}^\alpha \hat{a}_{i,\alpha}^\dagger \hat{a}_{j,\alpha} + \sum_{i,\alpha} \left[ \frac{U_{\alpha\alpha}}{2} \hat{n}_{i,\alpha} (\hat{n}_{i,\alpha} - 1) + E_{\alpha}^p \hat{n}_{i,\alpha} \right] + \sum_{i,\alpha \neq \alpha'} (U_{\alpha\alpha'} \hat{n}_{i,\alpha} \hat{n}_{i,\alpha'} + \frac{U_{\alpha\alpha'}}{2} \hat{a}_{i,\alpha}^\dagger \hat{a}_{i,\alpha'}^\dagger \hat{a}_{i,\alpha} \hat{a}_{i,\alpha'}). \quad (1)$$

Here  $\hat{a}_{i,\alpha}^\dagger$  creates a bosonic particle in the orbital  $\alpha = p_x, p_y, p_z$  at site  $i$ ,  $\hat{n}_{i,\alpha} = \hat{a}_{i,\alpha}^\dagger \hat{a}_{i,\alpha}$ , and the sum is over nearest neighbors  $i, j$ . The tunneling matrix elements are given by  $t_{ij}^\alpha = - \int d\mathbf{r} w_i^\alpha(\mathbf{r})^* [-\hbar^2 \nabla^2 / 2m + V(\mathbf{r})] w_j^\alpha(\mathbf{r})$  where  $w_i^\alpha(\mathbf{r})$  is the Wannier function of orbital  $\alpha$  at site  $i$ . Note that  $t_{ij}^\alpha$  is anisotropic. For instance, a boson in the  $p_x$ -orbital has a much larger tunneling rate in the  $x$ -direction than in the  $y$ -direction. The coupling constants are given by  $U_{\alpha\alpha'} = U_0 \int d\mathbf{r} |w_i^\alpha(\mathbf{r})|^2 |w_i^{\alpha'}(\mathbf{r})|^2$ , with  $U_0 (> 0)$  the onsite interaction strength determined by the scattering length. The last term in (1) is the orbital changing term describing the flipping of a pair of atoms from the state  $\alpha'$  to the state  $\alpha$ .

*Effective spin Hamiltonian.*— We are interested in the physics of the Mott insulator phase with unit filling in the strongly repulsive limit  $|t_{ij}^\alpha|^2 \ll U_{\alpha\alpha'}$ . Projecting onto the Mott space of singly occupied sites with the operator  $\hat{P}$ , the Schrödinger equation becomes  $\hat{H}_{\text{Mott}} \hat{P}|\psi\rangle = E \hat{P}|\psi\rangle$  with  $\hat{H}_{\text{Mott}} = -\hat{P} \hat{H} (\hat{H}_Q - E)^{-1} \hat{H} \hat{P}$ . Here  $\hat{Q} = 1 - \hat{P}$  and  $\hat{H}_Q = \hat{Q} \hat{H} \hat{Q}$  [14, 15]. Since we will find that  $E \sim t^2/U$ , we can take  $(\hat{H}_Q - E)^{-1} = \hat{H}_Q^{-1}$ .

For 2D, the space of doubly occupied states of a given site  $j$  is three-dimensional and spanned by  $|p_x p_x\rangle = 2^{-1/2} \hat{a}_{jx}^\dagger \hat{a}_{jx}^\dagger |0\rangle$ ,  $|p_y p_y\rangle = 2^{-1/2} \hat{a}_{jy}^\dagger \hat{a}_{jy}^\dagger |0\rangle$ , and  $|p_x p_y\rangle = \hat{a}_{jx}^\dagger \hat{a}_{jy}^\dagger |0\rangle$ . In this space, it is straightforward to find  $\hat{H}_Q$  from (1), and subsequent inversion yields

$$\hat{H}_Q^{-1} = \begin{pmatrix} U_{yy}/U^2 & -U_{xy}/U^2 & 0 \\ -U_{xy}/U^2 & U_{xx}/U^2 & 0 \\ 0 & 0 & 1/2U_{xy} \end{pmatrix} \quad (2)$$

with  $U^2 = U_{xx}U_{yy} - U_{xy}^2$ . Using (2) we can now calculate all possible matrix elements of  $\hat{H}_{\text{Mott}}$  in the Mott space. After some algebra we find

$$\begin{aligned} \hat{H}_{\text{Mott}} = & - \sum_{ij,\alpha} \left( \frac{2|t_{ij}^\alpha|^2 U_{\alpha\bar{\alpha}}}{U^2} \hat{n}_{i,\alpha} \hat{n}_{j,\alpha} + \frac{|t_{ij}^\alpha|^2}{2U_{xy}} \hat{n}_{i,\alpha} \hat{n}_{j,\bar{\alpha}} \right. \\ & \left. - \frac{2t_{ij}^x t_{ji}^y U_{xy}}{U^2} \hat{a}_{i,\alpha}^\dagger \hat{a}_{i,\bar{\alpha}} \hat{a}_{j,\alpha}^\dagger \hat{a}_{j,\bar{\alpha}} + \frac{t_{ij}^x t_{ji}^y}{2U_{xy}} \hat{a}_{i,\alpha}^\dagger \hat{a}_{i,\bar{\alpha}} \hat{a}_{j,\bar{\alpha}}^\dagger \hat{a}_{j,\alpha} \right) \end{aligned} \quad (3)$$

where  $\bar{x} = y$ , and  $\bar{y} = x$ . By further employing the Schwinger angular momentum representation,  $\hat{S}_i^z = \frac{1}{2}(\hat{a}_{xi}^\dagger \hat{a}_{xi} - \hat{a}_{yi}^\dagger \hat{a}_{yi})$ ,  $\hat{S}_i^+ = \hat{S}_i^x + i\hat{S}_i^y = \hat{a}_{xi}^\dagger \hat{a}_{yi}$  and  $\hat{S}_i^- = \hat{S}_i^x - i\hat{S}_i^y = \hat{a}_{yi}^\dagger \hat{a}_{xi}$ , together with the constraint  $\hat{a}_{xi}^\dagger \hat{a}_{xi} + \hat{a}_{yi}^\dagger \hat{a}_{yi} = 1$ , we can (ignoring irrelevant constants)

map (3) onto a spin-1/2 XYZ model in an external field

$$\hat{H}_{XYZ} = \sum_{\langle ij \rangle} J_{ij} \left[ (1 + \gamma) \hat{S}_i^x \hat{S}_j^x + (1 - \gamma) \hat{S}_i^y \hat{S}_j^y \right] + \sum_{\langle ij \rangle} \Delta_{ij} \hat{S}_i^z \hat{S}_j^z + h \sum_i \hat{S}_i^z. \quad (4)$$

Here,  $\langle i, j \rangle$  means summing over each nearest neighbor pair  $i, j$  only once. The couplings are given by  $J_{ij} = -2t_{ij}^x t_{ji}^y / U_{xy}$ ,  $\gamma = -4U_{xy}^2 / U^2$ , and  $\Delta_{ij} = -4(|t_{ij}^x|^2 U_{yy} + |t_{ij}^y|^2 U_{xx}) / U^2 + (|t_{ij}^x|^2 + |t_{ij}^y|^2) / U_{xy}$ . The magnetic field is  $h = 4 \sum_{\langle ij \rangle} (|t_{ij}^y|^2 U_{xx} - |t_{ij}^x|^2 U_{yy}) / U^2 + E_{p_x} - E_{p_y}$ , where  $E_\alpha$  is the onsite energy of the orbital  $\alpha$ . Note that  $t_{ij}^x t_{ji}^y < 0$  for  $p$ -band bosons [9] and therefore  $J_{ij} > 0$ . Also since  $|\gamma| < 1$ , the interactions between the  $y$ -component of neighboring spins favor anti-ferromagnetic order. As we shall see below, the sign of the couplings for interactions between the spin components  $x$ - and between  $z$ -, as well as the relative strength of all couplings can be experimentally controlled.

Equation (4) is a main result of this paper. It demonstrates how  $p$ -orbital bosons in a 2D optical lattice can realize the XYZ quantum spin-1/2 Heisenberg model. The fact that  $\gamma \neq 0$  is a consequence of the orbital changing term in (1), and it implies that the continuous  $U(1)$  symmetry for  $\hat{S}^x$  and  $\hat{S}^y$  is broken down to a set of  $Z_2$  symmetries. The  $Z_2$  symmetries reflect the ‘parity’ conservation in the original bosonic picture which classifies the many-body states according to total even or odd number of atoms in the  $p_x$ - and  $p_y$ -orbitals. We emphasize that this derivation makes no assumptions regarding the geometry of the 2D lattice - i.e. it can be square, hexagonal etc.

To illustrate the rich physics of the XYZ model and to examine finite size effects, we now focus on the case of a 1D lattice where we can obtain a reliable numerical solution of (4), and where quantum fluctuations are strong. Note that by increasing both the lattice amplitude and spacing in the  $y$ -direction keeping  $V_y k_y^2 \simeq V_x k_x^2$ , one can exponentially suppress tunneling in the  $y$ -direction to obtain a 1D model, while the  $p_x$  and  $p_y$  orbitals are still quasi-degenerate [16]. In the 1D setting, we will drop the “direction” subscript  $ij$  on the coupling constants.

For 1D, the importance of the orbital changing term can be further illuminated by employing the Jordan-Wigner transformation  $\hat{S}_i^- = e^{i\pi \sum_{j=1}^{i-1} \hat{c}_j^\dagger \hat{c}_j} \hat{c}_i$  for fermionic operators  $\hat{c}_i$  to the spin chain. The result is the fermionic Hamiltonian

$$\begin{aligned} \hat{H}_K / J = & \sum_n \left[ (\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{c}_{n+1}^\dagger \hat{c}_n) + \gamma (\hat{c}_n^\dagger \hat{c}_{n+1}^\dagger + \hat{c}_{n+1} \hat{c}_n) + \right. \\ & \left. \frac{\Delta}{J} (\hat{c}_n^\dagger \hat{c}_n + 1/2) (\hat{c}_{n+1}^\dagger \hat{c}_{n+1} - 1/2) + \frac{h}{J} (\hat{c}_n^\dagger \hat{c}_n - 1/2) \right]. \end{aligned} \quad (5)$$

We see that  $\gamma \neq 0$  leads to a pairing term that typically opens a gap in the energy spectrum. Incidentally the

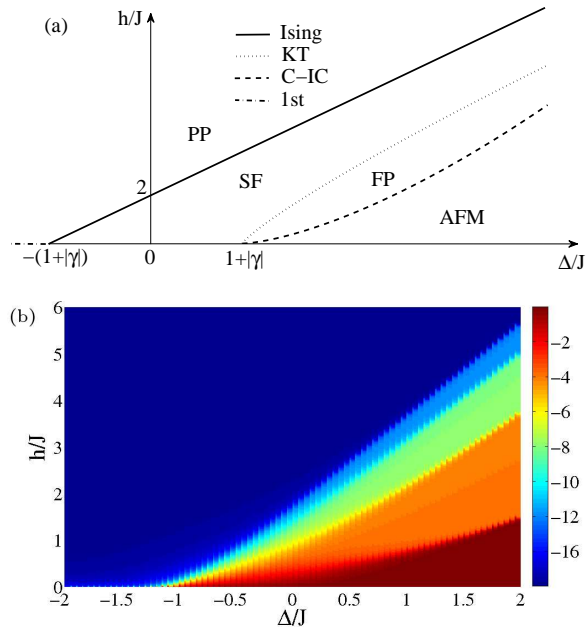


FIG. 1. (Color online) (a) Schematic phase diagram of the XYZ chain. (b) Finite size 'phase diagram' obtained by exact diagonalization of 18 spins. The finite size 'phase diagram' comprises an incomplete devil's staircase of SDW between the PP and AFM phases. As the system size is increased, the devil's staircase approaches the SF and the FP of (a). The anisotropy parameter is  $\gamma = 0.2$  in (b).

limit of  $\Delta \rightarrow 0$  in Eq. (5) is a realization of the Kitaev chain [17].

*XYZ phase diagram.*— We focus here on the most natural case for the implementation with  $p$ -orbital bosons, namely when the  $x$ - and  $y$ - components of spin favor anti-ferromagnetic ordering ( $|\gamma| < 1$ ). The schematic phase diagram is illustrated in Fig. 1 (a). At zero field, the XYZ model is integrable [18]. For large positive values of  $\Delta/J$  the system is anti-ferromagnetic (AFM) in the  $z$ -direction. Small values of  $\Delta/J$  are characterized by Néel ordering in the  $y$ -direction and the system is in the so-called spin-flop phase (SF). The  $h = 0$  line for large negative values of  $\Delta/J$  is characterized by a ferromagnetic phase (FM) in the  $z$ -direction, and for all the cases, the limit of large external field displays a magnetized phase (PP), where the spins align along the orientation of the field in the  $z$ -direction. These three phases also characterize the phase diagram of the XXZ model in a longitudinal field [19]. However, for non-zero anisotropy  $\gamma$ , a gapless floating phase (FP) emerges between the SF and the AFM phases which is characterized by power-law decay of the correlations [13, 20, 21]. The transition from the AFM to the FP is of the commensurate-incommensurate (C-IC) type whereas the transition between the FP and SF phases is of the Berezinsky-

Kosterlitz-Thouless (BKT) type. For  $\Delta < -(1 + |\gamma|)$  there is a first order transition at  $h = 0$  between the two polarized phases. Finally, there is an Ising transition between the PP and the SF phases.

*Finite size 'phase diagram'.*— The experimental realization of the Heisenberg model with cold atoms will inevitably involve finite size effects due to the harmonic trapping potential. Within the local density approximation, the trap renormalizes the couplings so that they become spatially dependent [22], but this effect can be negligible if the orbitals are small compared to the length scale of the trap. In the regime of strong repulsion, the main effect of the trap is instead that it gives rise to "wedding cake" structures with Mott regions of integer filling. This effect was observed in the lowest band Bose-Hubbard model [1], and predicted theoretically to occur for antiferromagnetic systems [23]. We therefore expect that for trapped systems, there will be finite Mott regions where the physics is controlled by the Heisenberg model as described in this paper.

To examine finite size effects, we have performed an exact diagonalization of a chain with 18 spins with open boundary conditions. Figure 1 (b) displays the resulting finite size 'phase diagram'. The colors correspond to different values of the total magnetization  $M = \sum_i \langle \hat{S}_i^z \rangle$  of the ground state. While the PP phase and the AFM phase are both clearly visible, the numerical results reveal a step like structure of the magnetization in between the two phases. We attribute these steps in  $M$  to a devil's staircase structure of spin-density-waves (SDW). Consider a system of  $L$  sites, open boundary conditions and fixed values of  $\gamma$  and  $\Delta > 1 + |\gamma|$ . Increasing the field from  $h = 0$ , the staggered magnetization experiences modulations until the system enters the PP. The system passes through a succession of plateaus with different values of total magnetization which build an incomplete devil's staircase [20]. As we see from Fig. 1 (b), the result is that it is only possible to give a numerical result for the PP-SF Ising transition. In particular, the C-IC and BKT transitions are overshadowed by the transitions between SDW. Larger values of  $L$  allow for a larger number of plateaus and thus to a larger number of SDW with different periodicities. In the thermodynamic limit the staircase becomes complete and the changes in  $M$  become smooth. One then recovers the phase diagram of Fig. 1 (a). These transitions, between different SDW, are more pronounced for moderate systems sizes. For a typical experimental system with  $\sim 50$  sites, for example, we estimate  $\sim 15$  different SDW between the AFM and PP phases.

*Measurements and manipulations.*— While time-of-flight measurements can reveal some of the phases [12], single-site addressing techniques [24] will be much more powerful when extracting correlation functions. To address single orbital states or even perform spin rotations, one may borrow techniques developed for trapped

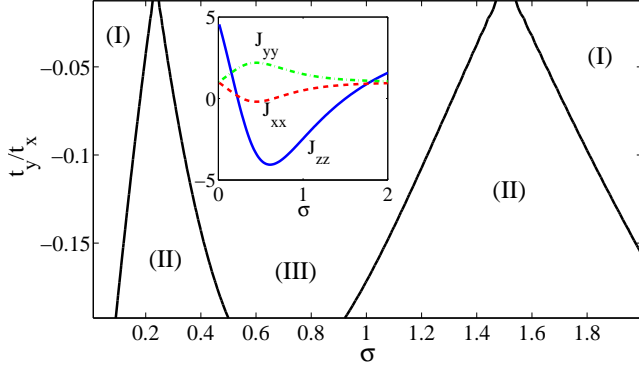


FIG. 2. (Color online) Different types of models are achieved by varying the relative tunneling strength and the relative orbital squeezing. The three different parameter regions are: (I) anti-ferromagnetic couplings in all spin components with  $\Delta > J(1 + |\gamma|)$ , (II) ferromagnetic or anti-ferromagnetic couplings in the  $z$ -component and anti-ferromagnetic in the  $y$ -component with  $J(1 + |\gamma|) > |\Delta|$ , and (III) same as in (II) but with  $|\Delta| > J(1 + |\gamma|)$ . The inset shows one example of the spin parameters  $J_{xx} = (1 + \gamma)$ ,  $J_{yy} = (1 - \gamma)$ , and  $J_{zz} = \Delta/J$  for  $t_y/t_x = -0.1$ .

ions [25]. Making use of the  $p_x$  and  $p_y$  orbitals symmetries, stimulated Raman transitions can drive both side-band and carrier transitions for the chosen orbitals in the Lamb-Dicke regime. These transitions can be made so short that the system is essentially frozen during the operation. Driving side-band transitions in this way, spin rotations may be implemented. For example, a rotation around  $x$  is achieved by driving the red-sideband for both orbitals and in the large detuned case an adiabatic elimination of the  $s$ -band results in the desired operation. Alternatively, Stark-shifting one of the  $p$ -orbitals results in a rotation around  $z$ . Since the spin operators do not commute, any rotation can be realized from these two operations. Performing fluorescence on single orbital states by driving the carrier transition acts as measuring  $\hat{S}_i^z$ . This combined with the above mentioned rotations makes it possible to measure the spin at any site in any direction.

*Tuning of couplings.*— For a square optical lattice, we have  $U_{xx} = U_{yy}$ . Moreover, in the harmonic approximation  $U_{xy} = U_{xx}/3$ , from which it follows that  $\Delta < 0$  and  $\gamma = -1/2$ . Thus, for a square lattice in the harmonic limit, interactions between the  $z$ -component of neighboring spins have ferromagnetic couplings, while the interactions between  $x$ - and between the  $y$ -components have anti-ferromagnetic ones. We now show how the relative strength and sign of the different couplings can be controlled by squeezing one of orbital states. Such squeezing can be accomplished by again driving the carrier transition of either of the two orbitals, dispersively with a spatially dependent field. The shape of the drive can be chosen such that the resulting Stark shift is weaker in the center of the sites, re-

sulting in a narrowing of the orbital. To be specific, assume that the ratio of the harmonic length scales of the  $p_x$  and  $p_y$  orbitals in the  $y$ -direction,  $\sigma$ , is tuned. A straightforward calculation using harmonic oscillator functions yields  $\alpha = U_{xx}/U_{xy} = 2^{-3/2}3(1 + \sigma^2)^{3/2}/\sigma$  and  $\beta = U_{yy}/U_{xy} = 2^{-3/2}3(1 + \sigma^2)^{3/2}$ . The coupling constants now depend on  $\sigma$  as  $\Delta/J = 2t^x(t^y)^{-1}\beta/(\alpha\beta - 1) + 2t^y(t^x)^{-1}\alpha/(\alpha\beta - 1) - (t^x/t^y + t^y/t^x)/2$  and  $\gamma = -4/(\alpha\beta - 1)$ . The inset in Fig. 2 displays the three coupling parameters as a function of  $\sigma$  for  $|t^x/t^y| = 0.1$ . We see that the relative size and even the sign of the couplings can be tuned by varying  $\sigma$ . In particular, while  $\hat{S}_y$  always has AFM couplings, they can be made both FM or AFM for  $\hat{S}_x$  and  $\hat{S}_z$ . In the main part of Fig. 2, we sketch the different accessible models as a function of  $t^y/t^x$  and  $\sigma$ . This clearly demonstrates that one can realize a whole class of XYZ spin chains by using this method.

*Experimental realization.*— In Ref. [11], the experimental realization of  $p$ -band bosons with a lifetime of several milliseconds was reported. With an average number of approximately two atoms per site, the atoms could tunnel hundreds of times in the  $p$ -band before decaying. The main decay mechanism was atom collisions [9]. When there is only one atom per site, an increase in the lifetime is therefore expected and corresponds to a factor of five longer [11]. Typical values of the couplings can be estimated from the overlap integrals of neighboring Wannier functions. Taking  $^{87}\text{Rb}$  atoms and  $\lambda_{\text{lat}} = 843\text{nm}$ , we have  $J/E_R \simeq 0.1$  with  $E_R = \hbar^2 k^2/2m$ , and the characteristic tunneling time is  $\tau = \hbar/JE_R \sim 500 \mu\text{s}$ . This is a few hundred of times smaller than the expected life-times [11] which allows for the experimental explorations of our results. Furthermore, the spin correlations we discuss in this paper will emerge for temperatures  $k_B T \lesssim J \sim t^2/U$ . This is the usual temperature scale for spin models based on exchange couplings [7].

*Conclusions.*— We showed that the Mott regime of unit filling of bosonic atoms in the first excited band of an optical lattice realize the spin-1/2 XYZ quantum Heisenberg model. We then illustrated the rich physics of this model by examining the phase diagram of the 1D case. Finite size effects relevant to the trapped systems were shown to give rise to spin-density-waves and a devil's stair case structure. We proposed a method to control the strength and relative size of the spin couplings thereby demonstrating how one can realize a whole class of XYZ models. In this respect, the system is a promising candidate for simulations of quantum magnetism. We finally discussed experimental issues related to the realization of this model. We end by noting that an exciting prospect is the 3D case, where we expect the three orbital model to result in even richer physics.

*Acknowledgments.*— We thank Alexander Altland, Alessandro De Martino, Henrik Johansson, Stephen Powell, and Eran Sela for helpful discussions. We acknowl-



edge financial support from the Swedish research council (VR). GMB acknowledges financial support from NORDITA.

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